Sensitivity Analysis Of Autoignition Simulation At Gas Turbine Operating Conditions

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The demand to reduce CO_2 emissions favors the use of alternative hydrogen-rich fuels, which can stem from pre-combustion carbon capture or power-to-gas technologies. These fuels are characterized by a higher reactivity and reduced ignition delay time compared to natural gas. Therefore, current combustor designs need to be adapted to the new requirements. Numerical modeling greatly assists the further development of such systems. The present study aims to determine how far a sophisticated combustion CFD method is able to predict autoignition at real engine conditions. Scale-resolving computations of autoignition were performed at elevated pressure (15 bar) and intermediate temperatures ($>$ 1000 K). The conditions are similar to those occurring in premixing ducts of reheat combustors. A nitrogen-diluted hydrogen jet is injected perpendicularly into a stream of hot vitiated air. The scale-adaptive simulation method (SAS) as proposed by Menter and co-workers has been applied. The chemistry is captured by direct inclusion of detailed kinetics. Subgrid fluctuations of temperature and species are considered by an assumed probability density function (PDF) approach. The results are compared with appropriate experimental reference data. The focus of the present work is set on the identification of the major sources of uncertainty in the simulation of autoignition. Despite the very challenging operating conditions, satisfactory agreements could be obtained within experimental uncertainties.

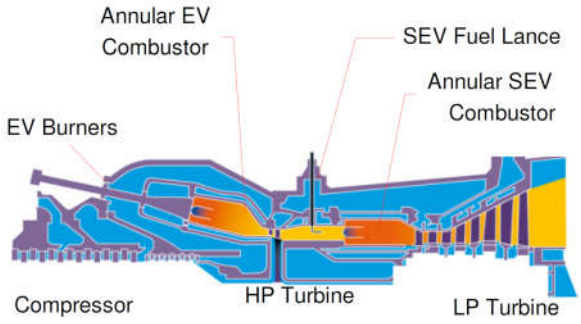

Fig. 1. Alstom GT24/GT26 gas turbine [1]

Nomenclature

RANS Reynolds-Averaged Navier-Stokes
SAS Scale-Adaptive Simulation
LES Large Eddy Simulation
EV EnVironmental (First) Combustor
MS Mixing Section
PDF Probability Density Function
SEV Sequential EnVironmental (Second) Combustor
TCI Turbulence-Chemistry Interaction

1 Introduction

In modern stationary gas turbines fuel and air are partially premixed upstream of the combustion chamber to ensure low NO_x emissions. Sufficient mixing must be achieved within the premixing duct. However, the residence time is limited by the ignition delay time of the combustible mixture. In the present study autoignition processes in the mixing region of reheat systems are investigated (Fig. 1). Sequential combustion systems allow high efficiency, flexibility and low emissions. Compressed air is heated up in a first combustion stage (EV: EnVironmental Combustor) and is partially expanded in a high-pressure (HP) turbine. In a sequential combustion stage (SEV), additional fuel is injected and mixed with the exhaust gas before it is burned in the reheat combustor. The temperature of the exhaust from the first stage lies above 1000 K. This system is successfully implemented in the ALSTOM GT24 and GT26 family [2]. Alstom's sequential combustion system is operating reliably for almost 20 years. During this time much experience has been gained with the application of natural gas.

The demand to reduce CO_2 emissions favors the use of alternative hydrogen-rich fuels. These fuels are characterized by a high reactivity, which leads to shorter ignition delay times and tightened flashback margins compared to conventional fuel. Current combustor designs need to be adapted to the new requirements [1]. A reliable prediction of autoignition is necessary to ensure safe operation.

In most technical applications, such as steady premixed combustion or diffusion flames, chemical and turbulent time scales are of different magnitude. Therefore, many established combustion models are based on scale separation of chemistry and turbulence. Autoignition in turbulent non-premixed flows, on the other hand, is governed by similar chemical and turbulent scales with strong interaction of both. Advanced numerical simulation tools are required to capture the underlying effects.

In literature a number of different modeling approaches for autoignition simulation in turbulent flows can be found. Almost all proposed methods are validated against laboratory-scale experiments at atmospheric pressure, e.g. [3–5]. However, gas turbine combustion is characterized by high pressure conditions. Extrapolating the combustion models to technically relevant conditions might be critical, especially for hydrogen-rich fuels. In the application domain of interest, hydrogen autoigniton can be controlled by two different chemical pathways. The crossover between the two pathways depends mainly on pressure and temperature [6,7]. Studies on ignition in non-premixed counterflows have shown that ignition below crossover is much more sensitive towards strain than for conditions above crossover [8,9]. Dependent on the surrounding conditions, the numerical prediction of autoignition can be more or less sensitive towards uncertainties in the turbulence-chemistry-interaction models and kinetic mechanisms.

The current study aims at determining the capabilities and main sources of uncertainty in the prediction of autoignition at engine operating conditions.

The numerical results are compared with appropriate high pressure experiments, which were conducted at the German Aerospace Center (DLR) in previous studies [10].

Quantification of uncertainties in both experimental measurements and numerical simulation is necessary to state whether any disagreement between model and experiment is due to modeling assumptions or is within the range of experimental uncertainties [11].

The next two sections deal with the description of the experimental reference data and the computational solution. In the following part different sources of uncertainties in the prediction of autoignition are evaluated by parameter variations. First, uncertainties due to different computational submodels are quantified. Then the uncertainties in input parameters, such as temperature and composition at the inflow boundary are estimated and their impact on the solution is evaluated.

2 Experimental Reference Data

Detailed experimental investigation of autoignition at gas turbine relevant conditions was conducted at DLR in previous studies. This section gives a short overview of the respective experimental reference data, which is used to validate the computational solution. A detailed description of the experiment and further data can be found in Fleck et al. [10, 12].

The experimental configuration is shown in Fig. 2. The upstream part consists of a hot gas generator and a supply of fresh dilution air, which resembles the cooling of the high pressure turbine. In the subsequent duct, emission and temperature probes are mounted and a nitrogen-diluted hydrogen jet is injected perpendicularly into the hot vitiated air. The mixing region is optically accessible. Potential autoignition events can be detected by luminescence measurements. Downstream, the sequential "reheat" combustion chamber (SEV) is attached to mixing section.

The pressure in the mixing section is set to 15 bar. The hot vitiated air has a velocity of 200 m/s, a temperature above 1000 K and an oxygen molar fraction of approximately 15 vol%. To keep the system simple and the modeling cost affordable, a fuel mixture of pure hydrogen and nitrogen was chosen for a first assessment. Mixtures of natural gas with hydrogen will be investigated in subsequent studies. The fuel jet has a velocity of 140 m/s and a hydrogen

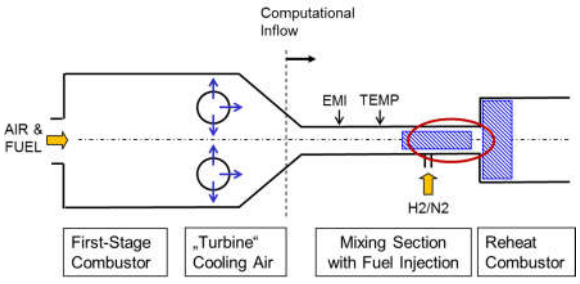

Fig. 2. Experimental setup [10]

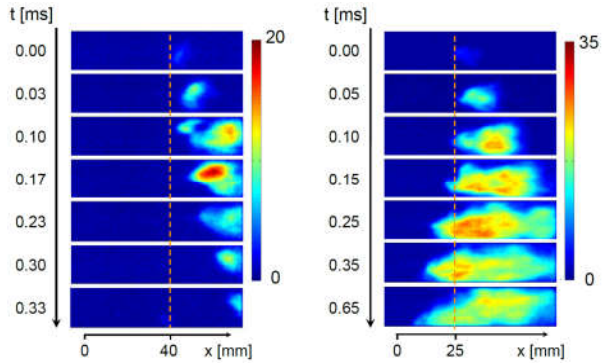

Fig. 3. Luminescence signal of autoignition events [10], left: non-stabilizing ignition kernel, right: stabilizing ignition kernel

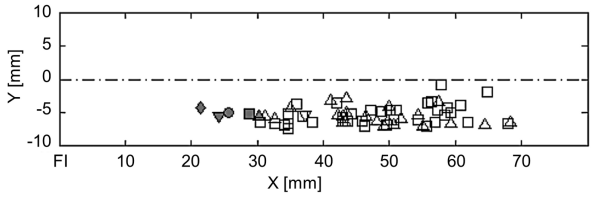

Fig. 4. Position of ignition kernels [10]

content of 31 vol%. The residence time in the mixing region is about 0.5 ms.

Figure 3 shows the temporal evolution of two exemplary ignition events, which were detected by luminescence measurements. The axis origin is set to the fuel injection. In the example on the left side an ignition kernel appears for the first time at about 40 mm. It increases in extent and intensity while it moves downstream towards the exit until it is flushed out of the mixing section. A couple of such ignition events were observed during one test run. The positions of the first kernel occurrences are plotted in Fig. 4 for different test runs. Each symbol represents one run. It is obvious that the positions vary extensively and are scattered across the whole mixing region. Kernels, which appeared downstream of 30 mm were flushed out (open symbols). The closed symbols correspond to kernels with the shortest ignition delay time of the respective run. These ignition spots started to advance upstream towards the fuel injection and led to flame stabilization in the recirculation zone (Fig. 3 right) [13].

3 Computational Solution

Based on the experimental conditions a numerical simulation was conducted. This served as reference solution for the subsequent sensitivity study.

3.1 Methodology

The simulations were conducted with the DLR in house code THETA (Turbulent Heat Release Extension of the TAU Code). This is a pressure-based CFD solver, which was developed for the simulation of flows with chemical reaction in combustion chambers.

The turbulence is modeled by the scale-adaptive simulation (SAS) approach as proposed by Menter et al. [14]. Previous studies have shown that important features of the recirculation zone and the associated flame stabilization can only be captured by scale-resolving methods [15]. Due to the large Reynoldsnumber of 10^5, pure Large-Eddy Simulation (LES) is not feasible. Therefore hybrid LES/RANS modeling gives the best compromise between accuracy and cost for the present application.

The chemistry is captured by direct inclusion of detailed kinetic mechanisms. Additional transport equations are solved for 9 species and enthalpy. The molecular viscosity and thermal diffusivity are determined as functions of temperature and composition, whereas species diffusivities are derived from a unity Lewis number assumption. The turbulent subgrid species and enthalpy fluxes are closed by a gradient transport hypothesis using constant turbulent Prandtl and Schmidt numbers. The chemical source term is modeled directly by the Arrhenius equation with reaction constants taken from the mechanism of Ó Conaire [16]. Using the cell averaged temperature for the computation of the source term could lead to large errors due to the non-linearity of the chemical reaction rate. Therefore a turbulence-chemistry interaction (TCI) model is required to account for the unresolved subgrid fluctuations. The expectation of the chemical source term is determined by applying assumed joint probability density functions (PDF) for species and temperature. A clipped-Gaussian PDF is applied for temperature and a statistically independent multivariate beta-PDF for the species. The required moments are determined by additional transport equations. A detailed description of the approach can be found in Gerlinger et al. [17, 18]. The model was successfully applied to the simulation of hydrogen autoignition in an atmospheric lab-scale burner by Di Domenico [19].

The simulation domain comprises the mixing duct and the sequential combustion chamber (SEV). The inflow boundary is chosen considerably far upstream of fuel injection to consider flow perturbations by the emission and temperature probes (Fig. 2). The SEV is also included to account for potential pressure and temperature fluctuations. The grid spacing in the mixing region is 0.8 mm. The total grid has about 1 million grid points. The wall cooling is approximated by isothermal wall boundaries at $T_{wall}/T_{hg} \approx 0.85$. Adiabatic conditions are applied for the temperature probe and the fuel pipe. The inflow streams are specified by the experimentally measured mass fluxes. The stream temperatures are assumed to be constant.

3.2 Results

A first solution is computed at experimental reference conditions. A snapshot of the temperature distribution in the mixing region is shown in Fig. 5. In contrast to the experiment no ignition can be observed in the simulation. Autoignition can only be reproduced when the temperature of the hot vitiated air T_{hg} is increased artificially. With an in-

crease of 10% the ignition occurs at about 60 mm (Fig. 6). A total temperature increase of 14% is necessary to achieve ignition at the same position as observed in the experiment (approx. 30 mm, Fig. 7).

In addition to this quantitative disagreement, there is also a qualitative difference. In the experiment, the positions of first kernel appearances are scattered along the whole region and kernels which appeared downstream of 30 mm are flushed out of the mixing section. However, in the computational results no isolated kernels are observed, but a steady flame with a stationary position far downstream of the recirculation region. Autoigniting kernels emerge permanently at the same location a few millimeters upstream of the stable lifted flame.

4 Sensitivity Analysis

The discrepancy between the experimental data and the simulation can arise from model deficiencies or be within the range of experimental uncertainties. To identify the most relevant uncertainty sources, a sensitivity analysis is performed. For a first assessment it is assumed that the different parameters are independent. The uncertainties due to different sources are measured by the shift of the averaged flame front position, which is defined by the maximum gradient of the averaged OH-concentration. Since no flame is present at the experimental reference temperature, the computation with an increased hot gas temperature of 10% serves as reference solution (Fig. 8). With an averaging interval of about 10 residence times, the flame front can be determined within an accuracy of 5 mm. The total deviation between experiment and simulation can also be expressed in flame front shift. The offset is more than 70 mm, since no ignition is present in the duct at the experimental reference temperature.

4.1 Model Form Uncertainties

The accuracy of the SAS turbulence model is dependent on the grid resolution, in a similar way as it is in LES. With increasing resolution more turbulence is directly resolved by the mesh and less turbulence must be modeled. Thus, the influence of the model is reduced when the grid is refined. The coarse grid (Fig. 8), used in the reference solution is refined two times. The medium grid (Fig. 9) has an average grid size of 0.4 mm in the mixing region, which is half the length in comparison to the reference grid. The fine grid (Fig. 10) has a grid size of 0.2 mm, which results in a grid point number of about 11 million. Figure 11 shows the eddy viscosity ratio for the three different grid resolutions. The ratio of the modeled turbulent viscosity ν_t to the molecular viscosity ν is a convenient quantity to assess the amount of

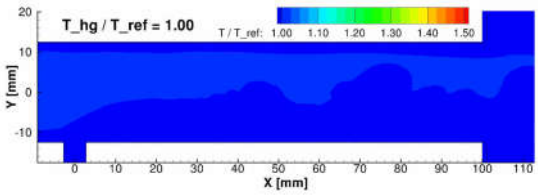

Fig. 5. Instantaneous temperature distribution for baseline hot gas temperature $T_{hg}/T_{ref} = 1.00$

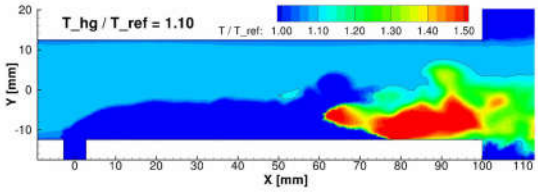

Fig. 6. Instantaneous temperature distribution for baseline hot gas temperature $T_{hg}/T_{ref} = 1.10$

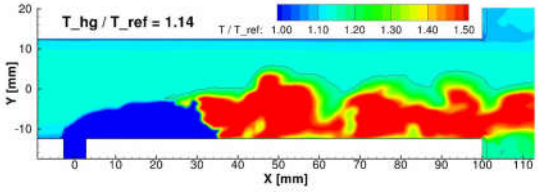

Fig. 7. Instantaneous temperature distribution for baseline hot gas temperature $T_{hg}/T_{ref} = 1.14$

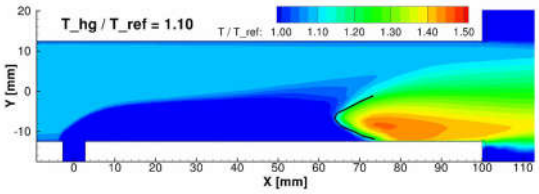

Fig. 8. Averaged temperature distribution for $T_{hg}/T_{ref} = 1.10$ with flame front on the coarse grid

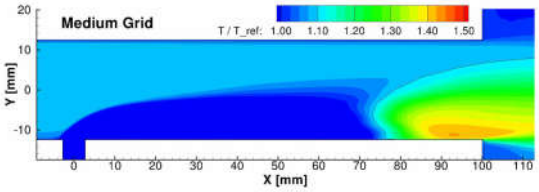

Fig. 9. Averaged temperature distribution for $T_{hg}/T_{ref} = 1.10$ on the medium grid

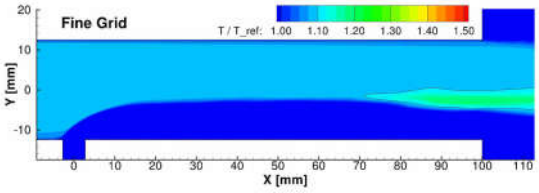

Fig. 10. Averaged temperature distribution for $T_{hg}/T_{ref} = 1.10$ on the fine grid

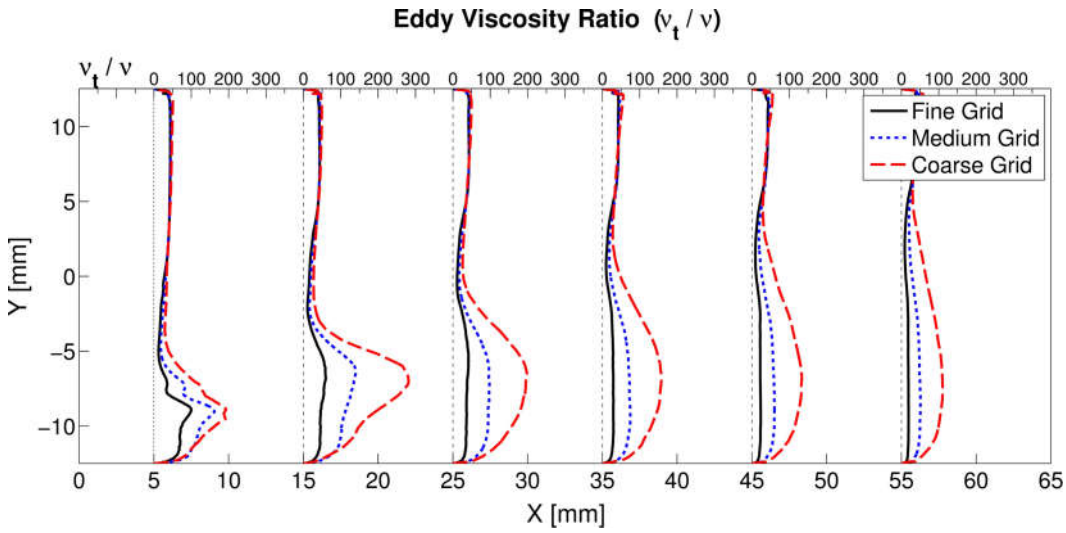

Fig. 11. Eddy viscosity ratio

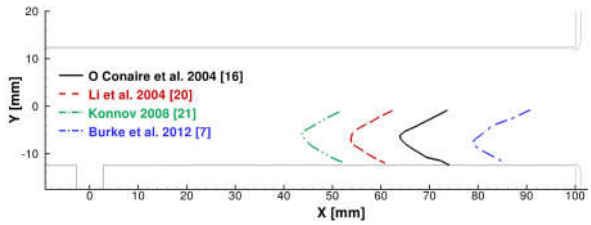

Fig. 12. Kinetic mechanisms

modeled turbulence. In the mixing region, the eddy viscosity ratio of the fine grid is about 5 times smaller compared to the coarse reference grid. It is apparent that the impact of the turbulence model is reduced significantly with grid refinement. The resulting effect on the flame is shown in Fig. 9 and 10. The distribution of averaged temperature varies significantly in its shape, but the position of the flame front varies only by about 8 mm.

In the computation of the reference solution the molecular viscosity and thermal diffusivity are calculated as functions of temperature and composition, whereas unity Lewis number is assumed for the species diffusivities. In hydrogen combustion this assumption can lead to larger uncertainties compared to other fuels, since hydrogen molecules and radicals are much more diffusive than other species. To evaluate the impact of this assumption, an additional computation was conducted with consideration of specific diffusivities. The flame front is shifted slightly upstream with an offset of less than 5 mm (Tab. 1).

The accuracy of the kinetic mechanism is estimated by comparison of competing models [7, 16, 20, 21]. The total difference in flame front position for time averaged results is 25 mm (Fig. 12). The models were previously compared to homogenous reactor and shock tube experiments [6, 7, 22, 23]. Homogenous ignition delay time calculations at similar test conditions have shown differences between recent hydrogen mechanisms of a factor of 2 [23]. This divergence is similar to the uncertainty observed in the present investigation.

Table 1. Uncertainties of computational submodels

Sub-Model	Methodology	Δx_{max} [mm]
Turbulence	Grid Refinement	8
Diffusivity	Le = 1 / Le (T, Y_i, p)	5
Chemistry	Competing Models	35
TCI	Model on / off	25

The influence of the assumed PDF-model is estimated by switching-off the complete model. This means that the cell-averaged values for temperature and composition are used for the calculation of the chemical source term. If turbulence-chemistry interaction (TCI) is completely neglected, autoignition is delayed. In the respective computation the flame front is shifted towards the exit by about 25 mm.

4.2 Input Parameter Uncertainties

An overview of the investigated input parameters is given in Tab. 2. These have been varied within the range of experimental uncertainties. The impact of these uncertainties on the flame front position is discussed in this section.

The composition of the hot vitiated air is recorded by an emission probe, which is located 180 mm upstream of the fuel injection (Fig. 2). Only the main species concentrations are measured, although intermediate species such as hydroxyl and hydrogen radicals can have an important ef-

Table 2. Effect of input parameter uncertainties

Parameter	Measurements	Method	Δx_{max} [mm]
Composition	Main Species	Intermediate Species & NO_x	5
Velocity	Massflow	Profile and Turbulence	5
Temperature	Thermocouple	see text	70

fect on the ignition delay time. The residence time in the first combustion chamber is approximately 30 ms. The time elapsing from the dilution with fresh air to the computational inlet is about 10 ms. This time is sufficient to reach chemical equilibrium considering pure hydrogen mechanisms with 9 species. The intermediate species concentrations were determined a by homogeneous reactor calculation and included in the computational setup of the inflow conditions. Moreover NO_x, which is not considered in the mechanism, can accelerate or prohibit ignition. The hydrogen mechanism of Ó Conaire [16] was extended with the NO_x chemistry by Mueller et al. [24]. A concentration of 100 ppm NO_x was applied at the inlet boundary. At high pressures, hydrogen combustion is not much affected by NO_x addition. Therefore it has only a minor effect at the present conditions. The resulting difference in the flame front position by including intermediate species and NO_x is less than 5 mm. This is in the order of the accuracy reached by averaging over 10 residence times.

The input stream velocities are derived from mass flow measurements. No turbulence quantities were measured. Different velocity profiles and turbulence intensities were applied in several simulations. The resulting shift in flame front position is minor.

The sensitivity towards uncertainties in hot gas temperature are assessed in two steps. First, uncertainties in the averaged temperature are estimated. In a second step temperature fluctuations are investigated. The temperature of the hot gas is measured by a shielded thermocouple in the center of the channel 100 mm upstream of the fuel injection (Fig. 2). It has a temporal resolution of 1 Hz and a standard deviation of about 1%. The hot gas is cooled between the thermocouple and the location of fuel injection due to wall cooling. The heat flux across the wall is estimated experimentally by the temperature increase of the coolant streams. In addition basic heat conduction calculations were performed. The resulting heat flux is applied to the wall boundaries. The total temperature offset between the two locations is determined by the computation and is about 0.2%. A total uncertainty of about 2% for the averaged temperature would result in a flame front shift of less than 2 mm.

More important than the averaged temperature is the local temperature maximum, since the shortest ignition delay time will occur at the highest temperature peak. Therefore, uncertainties in temperature fluctuations must be considered as well. The total range of temperature measurements varies by about 1% (Fig. 13). The temporal resolution of the thermocouple is 1/s. This is relatively coarse compared to the mixing section residence time of about 0.5 ms. Temperature fluctuations can be produced by combustion instabilities in the hot gas generator and by the injection of cold dilution air into the hot exhaust. Therefore, the computational domain was extended to include the upstream mixing of hot gas and cooling air. For a first estimation the exhaust gas at the new computational inflow is approximated by adiabatic flame temperature and constant velocity. An instant temperature distribution is shown in Fig. 14. Large fluctuations are obvious in the mixing duct. Figure 15 shows a snapshot of the temperature sequence in the simulation at the position of the temperature probe. In contrast to the measurement the computed temperature varies over a range of about 15%. The wavelength is in the order of 1 ms, which is sufficient to initiate autoignition. These high-frequent fluctuations cannot be resolved by the temperature probe (Fig. 13). Previous variations of inflow temperature in a similar range (Fig. 5-7) suggest a possible spread of the flame front position in the order of 70 mm and more.

The large temperature interval leads to a broad range of ignition delay times and therefore a broad distribution of ignition kernels. In the experiment kernels occurred along the whole optically accessible area. Hot temperature peaks are followed by colder patches, so that kernels which occur downstream of the recirculation zone are transported out of

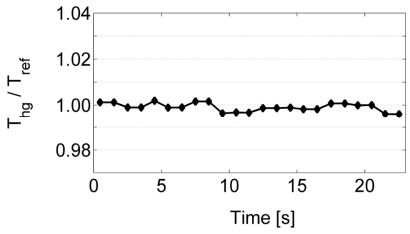

Fig. 13. Measured temperature signal [10]

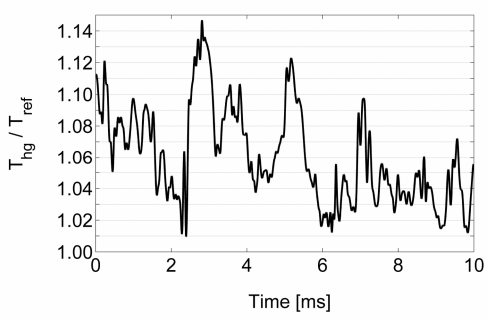

Fig. 15. Computed temperature signal at position of temperature probe

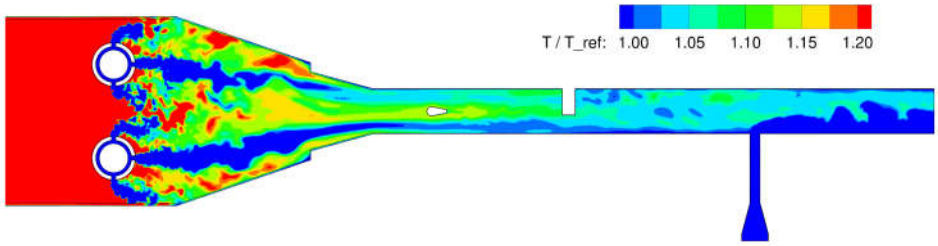

Fig. 14. Instantaneous temperature distribution for extended domain

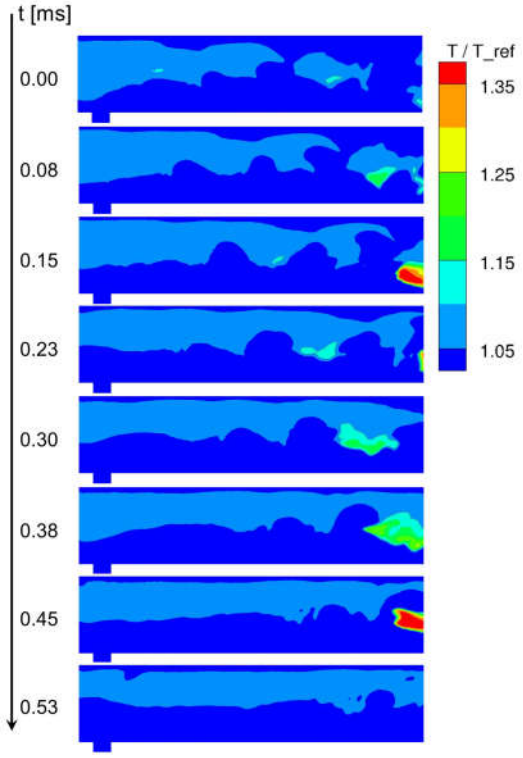

Fig. 16. Computation of ignition kernel evolution in the mixing duct with inclusion of hot gas temperature fluctuations

the mixing section. This cannot be captured by the simulation when a constant hot gas temperature is assumed. Whereas, when hot gas temperature fluctuations are considered in the simulation, the phenomenon of isolated kernels can be reproduced by the simulation (Fig. 16).

5 Conclusions

Numerical Simulations of hydrogen autoignition were conducted at conditions similar to those occurring in the premixing duct of gas turbine reheat combustors. The computational results were compared to experimental reference data. Discrepancies in the prediction of the autoignition time were observed in a quantitative as well as in a qualitative way. To assess and improve the predictive capability of the simulation, different sources of uncertainties were investigated and quantified. The most relevant uncertainty is due to temperature fluctuations in the hot vitiated air stream. Including the mixing of the hot gas with turbine cooling air into the computational domain shows that the fluctuations close to the fuel injection are in the order of 15%. Due to the challenging test conditions, the exact measurement of these fluctuations is limited. Additional simulations of the combustion in the first stage are necessary to determine the temperature fluctuations accurately. Further significant uncertainties are present in the modeling of the chemical source term. Competing kinetic mechanisms show large differences. The improvement of these mechanisms is still a topic of current research. The modeling uncertainty of the turbulence-chemistry interaction is of similar magnitude. However, switching-off the complete model is a fairly rough method to estimate the uncertainty. A more specific evaluation might help to further increase the confidence. In summary it is shown that the presented combustion model can predict autoignition at relevant reheat combustor conditions within the experimental uncertainties. The model is therefore a valuable tool in the development of fuel flexible gas turbine reheat burners.

Acknowledgements

The Jülich Supercomputing Centre is acknowledged for the computational time provided under the NIC project number 5904.

References

[1] Poyyapakkam, M., Wood, J., Mayers, S., Ciani, A., Guethe, F., and Syed, K., 2012. "Hydrogen combustion within a gas turbine reheat combustor". In ASME Turbo Expo 2012. Paper No. GT2012-69165.

[2] Joos, F., Brunner, P., Schulte-Werning, B., Syed, K., and Ergolu, A., 1996. "Development of the sequential combustion system for the ABB GT24/GT26 gas turbine family". In International Gas Turbine and Aeroengine Congress and Exhibition. Paper No. 96-GT-315.

[3] Jones, W., and Navarro-Martinez, S., 2007. "Large eddy simulation of autoignition with a subgrid probability density function method". *Combust. Flame,* **150**, pp. 170–187.

[4] Ihme, M., and See, Y. C., 2011. "LES flamelet modeling of a three-stream mild combustor: Analysis of flame sensitivity to scalar inflow conditions". *Proc. Combust. Inst.,* **33**, pp. 1309–1317.

[5] Stanković, I., Mastorakos, E., and Merci, B., 2013. "LES-CMC simulations of different auto-ignition regimes of hydrogen in a hot turbulent air co-flow". *Flow Turbul. Combust.,* **90**(3), pp. 583–604.

[6] Herzler, J., and Naumann, C., 2009. "Shock-tube study of the ignition of methane/ethane/hydrogen mixtures with hydrogen contents from 0% to 100% at different pressures". *Proc. Combust. Inst.,* **32**, pp. 213–220.

[7] Burke, M. P., Chaos, M., Ju, Y., Dryer, F. L., and Klippenstein, S. J., 2012. "Comprehensive H2/O2 kinetic model for high-pressure combustion". *Int. J. Chem. Kin.,* **44**, pp. 444–474.

[8] Fotache, C., Kreutz, T., Zhu, D. L., and Law, C. K., 1995. "An experimental study of ignition in non-premixed counterflowing hydrogen versus heated air". *Combust. Sci. Technol.,* **109**, pp. 373–393.

[9] Kreutz, T., and Law, C. K., 1996. "Ignition in non-premixed counterflowing hydrogen versus heated air: Computational study with detailed chemistry". *Combust. Flame,* **104**, pp. 157–175.

[10] Fleck, J., Griebel, P., Steinberg, A. M., Stöhr, M., Aigner, M., and Ciani, M., 2012. "Autoignition limits of hydrogen at relevant reheat combustor operating conditions". *ASME J. Gas Turb. Pwr.,* **134**, p. 041502.

[11] Najm, H. B., 2011. "Uncertainty quantification in fluid flow". In *Turbulent Combustion Modeling*, T. Echekki and E. Mastorakos, eds., Vol. 95 of *Fluid Mechanics and Its Applications*. Springer, Chapter 16.

[12] Fleck, J., Griebel, P., Steinberg, A., Stöhr, M., Aigner, M., and Ciani, M., 2010. "Experimental investigation of a generic, fuel flexible reheat combustor at gas turbine relevant operating conditions". In ASME Turbo Expo 2010. Paper No. GT2010-22722.

[13] Kolla, H., Grout, R. W., Gruber, A., and Chen, J. H., 2012. "Mechanisms of flame stabilization and blowout in a reacting turbulent hydrogen jet in cross-flow". *Combust. Flame,* **159**(8), pp. 2755–2766.

[14] Menter, F. R., and Egorov, Y., 2005. "A scale-adaptive simulation model using two-equation models". In 43rd AIAA Aerospace Sciences Meeting and Exhibit. Paper No. 2005-1095.

[15] Ivanova, E., Noll, B., Aigner, M., and Syed, K., 2012. "Numerical simulations of turbulent mixing and autoignition of hydrogen fuel at reheat combustor operating conditions". *ASME J. Gas Turb. Pwr.,* **134**, p. 041504.

[16] Ó Conaire, M., Curran, H. J., Simmie, J. M., Pitz, W. J., and Westbrook, C. K., 2004. "A comprehensive modelling study of hydrogen oxidation". *Int. J. Chem. Kin.,* **36**(11), pp. 603–622.

[17] Gerlinger, P., Möbus, H., and Brüggemann, D., 2001. "An implicit multigrid method for turbulent combustion". *J. Comput. Phys.,* **167**, pp. 247–276.

[18] Gerlinger, P., 2002. "Investigation of an assumed PDF approach for finite-rate chemistry". In 40th AIAA Aerospace Sciences Meeting and Exhibit. Paper No. 2002-0166.

[19] Di Domenico, M., 2007. "Numerical simulations of soot formation in turbulent flows". PhD thesis, Universität Stuttgart.

[20] Li, J., Zhao, Z., Kazakov, A., and Dryer, F. L., 2004. "An updated comprehensive kinetic model of hydrogen combustion". *Int. J. Chem. Kin.,* **36**, pp. 566–75.

[21] Konnov, A. A., 2008. "Remaining uncertainties in the kinetic mechanism of hydrogen combustion". *Combust. Flame,* **152**, pp. 507–528.

[22] Kéromnès, A., Metcalfe, W. K., Heufer, K. A., Donohoe, N., Das, A. K., Sung, C.-J., Herzler, J., Naumann, C., Griebel, P., Mathieu, O., Krejci, M. C., Petersen, E. L., Pitz, W. J., and Curran, H. J., 2013. "An experimental and detailed chemical kinetic modeling study of hydrogen and syngas mixture oxidation at elevated pressures". *Combust. Flame,* **160**(6), pp. 995–1011.

[23] Weydahl, T., Poyyapakkam, M., Seljeskog, M., and Haugen, N. E. L., 2011. "Assessment of existing H2/O2 chemical reaction mechanisms at reheat gas turbine conditions". *Int. J. Hydrogen Energy,* **36**(18), pp. 12025–12034.

[24] Mueller, M. A., Yetter, R. A., and Dryer, F. L., 1999. "Flow reactor studies and kinetic modeling of the H2/O2/NOx and CO/H2O/O2/NOx reactions". *Int. J. Chem. Kin.,* **31**, pp. 705–724.